Evaluation of a Scalar Probability Density Function Approach for Turbulent Jet Nonpremixed Flames

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Abstract

A scalar probability density function (PDF) method considering a detailed chemical kinetics is applied to a diluted hydrogen turbulent jet nonpremixed flame to evaluate the performance. The flame is formed on a nozzle of an inner diameter of D=6mm, with a fuel exit velocity of 30m/s, surrounded by two annular pipes issuing airs of higher and lower velocities of 30m/s and 3m/s, respectively. The hydrogen as a fuel is diluted by one third volumetrically by the nitrogen, giving a stoichiometric mixture fraction of 0.46. The flow field has been solved on the basis of the k-ε two equation model. A modelled scalar PDF equation has been solved by an Eulerian Monte Carlo method developed by Pope [1]. The PDF transport term due to turbulent velocity fluctuations involved in the PDF equation is modelled based on the gradient diffusion concept. The molecular mixing term is modelled by the modified Curl model. On the other hand, reactions are dealt exactly in the PDF method and a twenty-step reaction, eight species kinetic mechanism for hydrogen-oxygen combustion is employed here. Each joint scalar PDF is described as an ensemble of stochastic particles of thousand at each node. Each PDF is transported through each stochastic process of the turbulent diffusion, the molecular mixing, and the convection, and through the exact chemical reaction process. In order to evaluate the performance of the present PDF method, calculation results are compared with those of two flamelet calculations, which are the conventional laminar flamelet model method and a scalar PDF method based on the conserved scalar approach. The present PDF method can reproduce the extinction and re-ignition phenomena, which cannot be easily predicted by the conserved scalar approaches. Variations in the nonpremixed flame structure due to the flame stretch, which were experimentally confirmed by Barlow et al.[2], have been also reproduced.

1. Introduction

Modelling of turbulent combustion is challenging, because it always provides us difficult tasks to close modelled equations, referred to as the closure problem. Moment methods, which are now widely used, are suffered from an inevitable problem concerning reaction except for a minor problem of the velocity correlation terms. In usual turbulent combustion fields, the higher order fluctuation terms stemmed from the reaction term do not converge [3]. The laminar flamelet model resolves this problem on the basis of the conserved scalar concept which is built under the assumptions of fast chemistry and the unity Lewis number with equal diffusivities. In the model, scalar fluctuations are replaced by those of the mixture fraction. The flame stretch effect has been considered as an important factor in the model but the finite chemical reaction rate effect is not able to be dealt exactly. On the other hand, the probability density function (PDF) method has great advantages able to deal exactly with the reaction and the velocity correlation. The advantages are based on the characteristic which a one time, one point probability density function dealt in usual PDF approaches can have all

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information relating to both the processes of reaction and convection. The probability density function method is however required another modelling of diffusion processes caused by the spatial characteristics, such as the molecular mixing and the viscous momentum exchange. Many models are established for the molecular mixing [4]. The viscous momentum exchange is modelled in the Langevin equation [5]. In the present paper, a hybrid PDF method which consists of the moment method based on the k-ε two equation model for the flow field and a scalar PDF method for the scalar field respectively is discussed. Therefore, the modelling of the scalar PDF transport includes the turbulent velocity fluctuations and the molecular mixing processes.

In order to evaluate the prediction performance of the probability density function method considering a finite chemical reaction rate (F-PDF method), a diluted hydrogen turbulent jet nonpremixed flame was calculated by the F-PDF, the PDF method considering the infinite chemical reaction rate (I-PDF), and the flamelet model (F.M.) method, where the last two methods are based on the conserved scalar concept.

2. Numerical methodology

2.1 Scalar probability density function method

The present scalar PDF method is one of hybrid PDF methods. The scalar field is calculated by the PDF method, whereas the flow field is calculated by the moment method on the basis of the k-ε two equation model. Governing equations for the flow field are given in the cylindrical coordinate for coaxial flow, turbulent jet nonpremixed flames as follows:

Continuity equation:

$$\frac{\partial}{\partial x}(\bar{\rho}\tilde{u}) + \frac{1}{r}\frac{\partial}{\partial r}(r\bar{\rho}\tilde{v}) = 0 \tag{1}$$

Axial-momentum equation:

$$\bar{\rho}\tilde{u}\frac{\partial \tilde{u}}{\partial x} + \bar{\rho}\tilde{v}\frac{\partial \tilde{u}}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}(r\mu_{eff}\frac{\partial \tilde{u}}{\partial r}) \tag{2}$$

Turbulent kinetic energy transport equation:

$$\bar{\rho}\tilde{u}\frac{\partial k}{\partial x} + \bar{\rho}\tilde{v}\frac{\partial k}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}[r(\mu_l + \frac{\mu_t}{\sigma_k})\frac{\partial k}{\partial r}] + \mu_t\left(\frac{\partial \tilde{u}}{\partial r}\right)^2 - \bar{\rho}\varepsilon \tag{3}$$

Turbulent dissipation rate transport equation:

$$\bar{\rho}\tilde{u}\frac{\partial \varepsilon}{\partial x} + \bar{\rho}\tilde{v}\frac{\partial \varepsilon}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}[r(\mu_l + \frac{\mu_t}{\sigma_\varepsilon})\frac{\partial \varepsilon}{\partial r}] + C_{\varepsilon 1}\frac{\varepsilon}{k}\mu_t\left(\frac{\partial \tilde{u}}{\partial r}\right)^2 - C_{\varepsilon 2}\bar{\rho}\frac{\varepsilon^2}{k}\ , \tag{4}$$

where the effective viscosity $\mu_{eff} = \mu_t + \mu_l$, μ_t the turbulent viscosity, and μ_l the dynamic viscosity. The turbulent viscosity μ_t is given as

$$\mu_t = C_\mu f_\mu \frac{\rho k^2}{\varepsilon} \quad , \tag{5}$$

where f_μ is the correction factor for the decrease in the turbulent viscosity attributable to the laminarization in flames[6]. The constants C_μ, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, σ_k and σ_ε are ascribed the standard values 0.09, 1.44, 1.92, 1.0, and 1.3.

On the other hand, the modelled transport equation of mass density probability density function is given as

$$\tilde{u}\frac{\partial \tilde{P}(\underline{\psi})}{\partial x} + \tilde{v}\frac{\partial \tilde{P}(\underline{\psi})}{\partial r} + \frac{\partial}{\partial \psi_\alpha}\left(\tilde{P}(\underline{\psi})S(\underline{\psi})\right) = \frac{1}{\langle\rho\rangle}\frac{\partial}{r\partial r}\left(r\Gamma_T\frac{\partial \tilde{P}(\underline{\psi})}{\partial r}\right) + E(\underline{\psi};\underline{x}), \tag{6}$$

where ψ is the scalar independent variable and the underbar stands for a multicomponent. The mass density PDF $\tilde{P}(\underline{\psi})$ is defined as

$$\tilde{P}(\underline{\psi};\underline{x}) \equiv \rho(\underline{\psi})P(\underline{\psi};\underline{x})/\langle\rho\rangle \quad . \tag{7}$$

The first two terms on the left-hand side of Eq.(6) represent the transport by convection and the third term is that by reaction. The first term on the right-hand side represents the transport by the turbulent diffusion, modelled on the basis of the gradient diffusion concept. The last term represents the molecular mixing; the modified Curl model [7][8] is employed in the present study and is given as

$$E(\underline{\psi};x) = 2\beta\omega\int \widetilde{P}(\underline{\psi}+\underline{\psi}')\widetilde{P}(\underline{\psi}-\underline{\psi}')d\underline{\psi}' - 2\beta\omega\widetilde{P}(\underline{\psi}), \tag{8}$$

where β = 3 and the turbulent frequency ω is

$$\omega = C_\phi \frac{\varepsilon}{k} \quad . \tag{9}$$

The constant C_ϕ is ascribed the value 2.0. The coefficient Γ_T in the turbulent diffusion term of Eq.(6) is given as

$$\Gamma_T = \mu_{eff} / \sigma_\phi \quad , \tag{10}$$

where μ_{eff} is the effective viscous coefficient and σ_ϕ is the effective Schmidt number ascribed the value 0.7. The turbulent effective diffusivity is given by Γ_T / ρ.

The modelled scalar PDF transport equation (6) is solved by an Euler Monte Carlo method [1]. In the method, the computational domain is divided by a number of grids and the flow and the scalar fields are simultaneously solved on the same grids. Each PDF at each node is represented as an ensemble of fictional particles, scalar properties being assigned. Each process of the convection, the reaction, the turbulent diffusion, and the molecular mixing is dealt with as each fractional step. Each transport process of PDF is treated stochastically, with the exception of the reaction.

A joint scalar probability density function is described in a discrete manner as follows;

$$P_N(\underline{\psi};\underline{x},t) = \frac{1}{N}\sum_{n=1}^{N}\delta(\underline{\psi}-\underline{\phi}^{(n)}) \quad , \tag{11}$$

where ϕ is the eulerian scalar field and δ is the fine grained probability density function. The N is the total number of samples. A contineous PDF is described as the expected value of P_N as

$$P(\underline{\psi};\underline{x},t) = \left\langle P_N(\underline{\psi};\underline{x},t)\right\rangle \quad , \tag{12}$$

where the angled brackets indicate the ensemble average.

If the joint scalar PDF is obtained, the expectation of any function $Q(\underline{\psi})$ is estimated by the following relation.

$$\left\langle Q(\underline{\phi})\right\rangle = \int Q(\underline{V})P_N(\underline{\psi})d\underline{\psi} = \frac{1}{N}\sum_{n=1}^{N}Q(\underline{\phi}^{(n)}) \tag{13}$$

In the present study, two types of scalar PDF methods are employed; namely, one is the scalar PDF method considering the full chemical kinetics and the other considers the infinite chemical rate, referred to as F-PDF and I-PDF hereafter, respectively. The latter is based on the conserved scalar concept.

2.2 Flamelet model method

The conventional flamelet method is also employed to compare with the F-PDF method. The flamelet method requires the modelled transport equations of the mean mixture fraction $\widetilde{Z}$ and the variance $\widetilde{Z}''^2$ given as

$$\overline{\rho}\widetilde{u}\frac{\partial\widetilde{Z}}{\partial x} + \overline{\rho}\widetilde{v}\frac{\partial\widetilde{Z}}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_{eff}}{\sigma_Z}\frac{\partial\widetilde{Z}}{\partial r}\right) \quad , \tag{14}$$

$$\overline{\rho}\widetilde{u}\frac{\partial\widetilde{Z}''^2}{\partial x} + \overline{\rho}\widetilde{v}\frac{\partial\widetilde{Z}''^2}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\mu_{eff}}{\sigma_g}\frac{\partial\widetilde{Z}''^2}{\partial r}\right) + C_{g1}\mu_t\left(\frac{\partial\widetilde{Z}}{\partial r}\right)^2 - C_{g2}\overline{\rho}\frac{\varepsilon\widetilde{Z}''^2}{k} \quad , \tag{15}$$

where C_{g1} = 2.8 and C_{g2} = 1.92. The coefficients employed here are widely accepted. Note however that the modelled PDF equation (6) reproduces 2.85 and 2 for C_{g1} and C_{g2}, respectively. In flamelet calculations, PDFs are presumed as the clipped Gaussian profile in terms of $\widetilde{Z}$ and $\widetilde{Z}''^2$. The flamelet model is hereafter referred to as F.M.

2.3 Calculations

In order to evaluate the prediction performance of the F-PDF method, a turbulent jet nonpremixed flame of hydrogen/nitrogen was calculated by the F-PDF, the I-PDF, and the FM methods. The fuel is the mixture of hydrogen and nitrogen with a volumetric ratio of 1:2, giving a stoichiometric mixture fraction of 0.46. The fuel is issued from a round nozzle of i.d.=6mm surrounded by two annular air flows. Inner diameters of the annular air nozzles are 14mm and 140mm, respectively. The inside air nozzle is for the higher velocity air flow and the outside air nozzle for the lower velocity air flow. The exit velocity condition is a fuel velocity of 30m/s, a higher air flow velocity of 30 m/s, and a lower air flow velocity of 3 m/s.

The computational domain extends 60mm in the radial direction (r-direction) and 360mm in the axial direction (x-direction), respectively. The flow field was solved by the marching integration of finite difference equations. The modelled PDF equation is solved via the above-mentioned Monte Carlo method. Calculations are performed using a uniform grid size of 0.2 mm in the r-direction (grid number 300). One-thousand Monte Carlo particles are assigned at each grid. Predicted results in the present paper ensured irrespective of the grid size and a number of Monte Carlo particles. A full chemical mechanism of 9 species and 20 reactions for the reaction of hydrogen and oxygen was used in the F-PDF calculations. In the F-PDF method, a pilot flame, which consists of the burned gas of the stoichiometry, is used for the ignition in the range from r/R=1.0 to 1.6 at the exit of the burner, where R is the radius of the fuel nozzle..

3. Results and Discussion

In order to evaluate the performance of the present F-PDF method, calculation results are compared with those of two flamelet calculations (I-PDF and F.M.) on the basis of the conserved scalar approach. Figures 1 and 2 show a comparison of the flow fields among those calculations in terms of axial and radial velocities. Experimental data is also added to the figure, measured by a laser Doppler velocimetry. Every calculation shows good agreement with the experimental result and did not show any important differences among these methods. This close estimation for the flow field should permit us to discuss only about the scalar field.

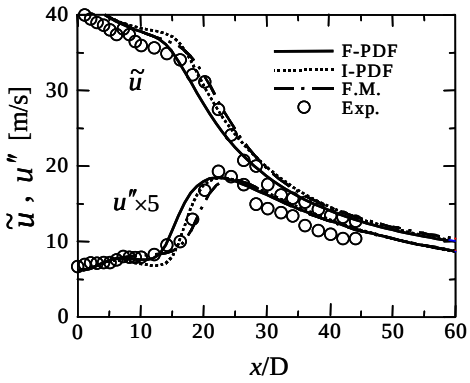


Fig.1 Axial Profiles of axial velocity and turbulent intensity along the center axis.

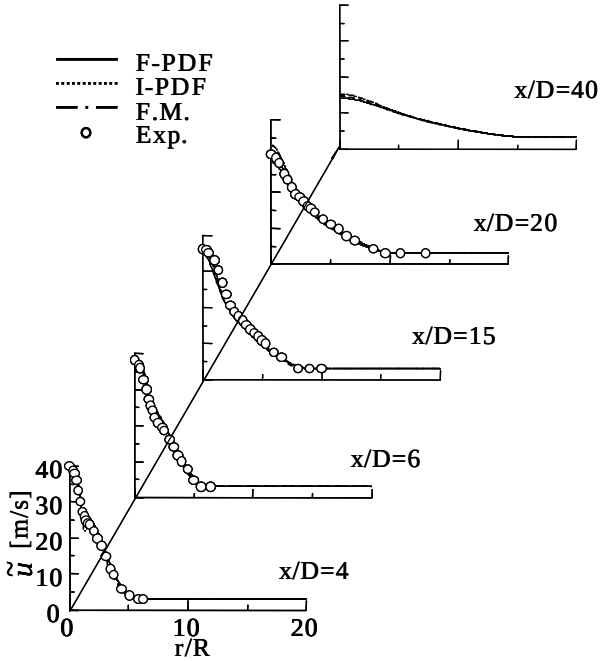


Fig.2 Radial profiles of axial velocity

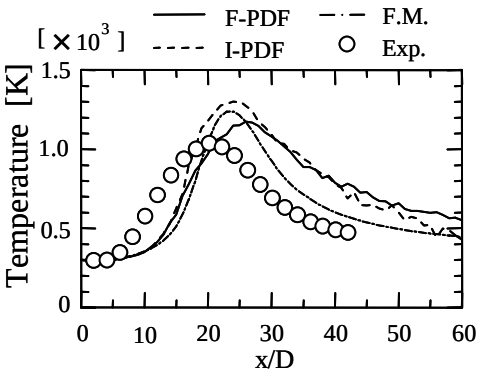


Fig.3 Axial profiles of temperature along the center axis.

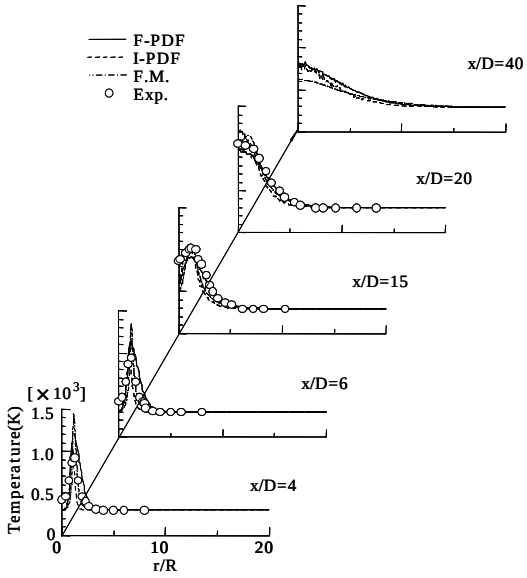
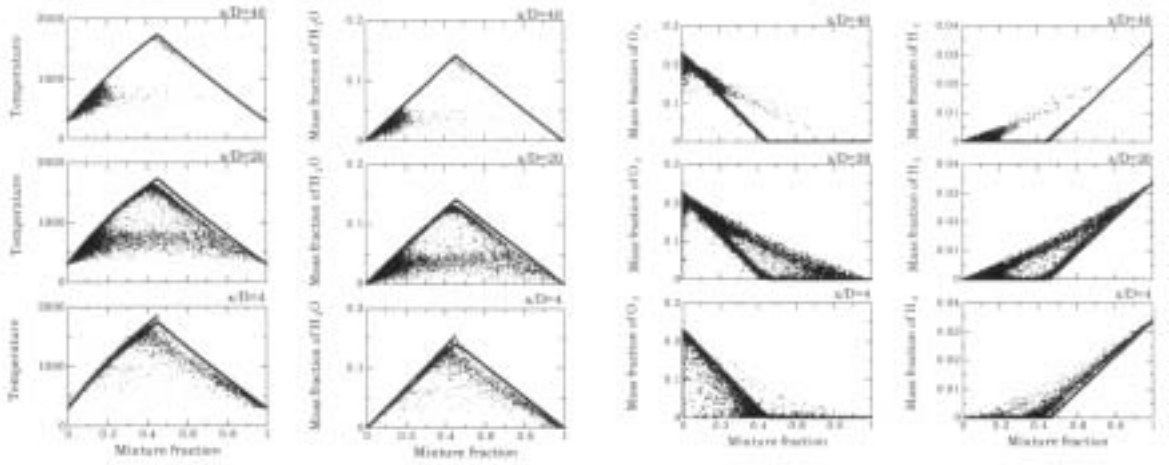


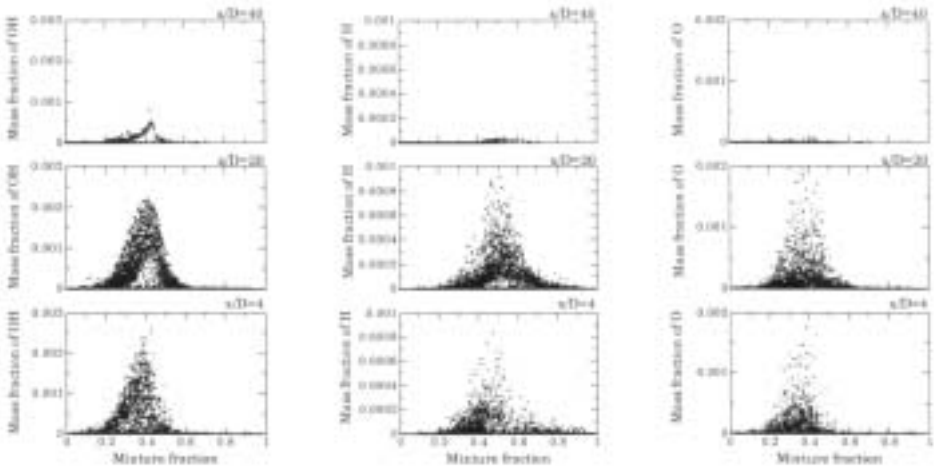
Fig.4. Radial profiles of temperature

Figures 3 and 4 show axial and radial profiles of temperature obtained by the three methods, respectively, together with experimental data measured by a thermocouple. Every calculation underestimates the temperature upstream on the center axis. This underestimation should be however attributable to the measurement of the thermocouple rather than the calculation methods. The thermocouple is affected by the radiation and the heat conduction; in this case, temperature is elevated due to the heat transfer from the flame surrounding the thermocouple. On the other hand, the maximum temperature is overestimated for every calculation. This difference is again caused by the measurement and attributable to the cooling of the thermocouple by the lower temperature ambient gas. The F-PDF method however has predicted the closer maximum temperature on the center axis to the experimental one than the other methods. This improvement should reflect the finite chemical rate considered only in the F-PDF method. The temperatures downstream of the maximum temperature position estimated by both the PDF methods have been overestimated due to the underestimation of mixing [9]. For the radial profiles of temperature, the calculation results are in good agreement with the experimental results, except for the maximum temperature in the near field to the nozzle.

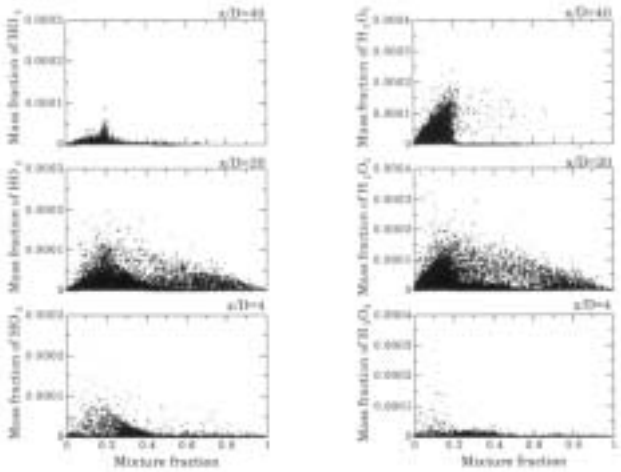
The prediction ability of the F-PDF method is highlighted in scatter plots of scalar quantities like temperature and species mass fractions shown in Fig.5. Solid lines in Figs.5(a) to (d) correspond to the flame structure under the assumption of the infinite reaction rate and one-step irreversible reaction. At x/D=4, scatter plots of the temperature and the main species of H_2O, O_2 and H_2 gather close to the solid lines with slight departures on the rich side. These slight departures may reflect the burning under the flame stretch supported by the pilot flame installed around the fuel nozzle, because the departures on the rich side from the flame structure of the infinite chemical rate and one-step irreversible reaction are found as caused by the flame stretch [2]. At x/D=20, the scatter plots collapse into around two regions of the above mentioned flame structure and of the frozen structure indicated by the straight lines connecting the properties of the fuel and the air before the mixing. The scatter plots around the frozen structure indicate local extinction due to the flame stretch at the location where the support of the pilot flame is weakened. This phenomenon is recognized as bimodal PDFs conditioned on the mixture fraction [10]. At x/D=40, the scatter plots again gather to around the fully burning limits, reflecting re-ignition after the local extinction at the upstream. Moreover, the deviations from the solid lines on the rich side gradually decrease with increasing x. This decrease shows the damping of the flame stretch with x. These results agree qualitatively with experimental results [11]. Consequently, the present PDF method can reproduce the extinction and re-ignition phenomena, which cannot be easily predicted by the conserved scalar approaches (F.M. and I-PDF



(a) T (b) H_2O (c) O_2 (d) H_2



(e) OH (f) H (g) O



(h) HO_2 (i) H_2O_2

Fig.5 Scatter plots of temperature and mass fractions of species. Solid lines in (a) to (d) correspond to the flame structure of one-step irreversible reaction.

methods). The variations in the diffusion flame structure on the rich side due to the flame stretch, which were experimentally confirmed by Barlow et al. [2], have been also reproduced. Moreover, Fig. 5 also shows scatter plots relating to the intermediate species of OH, H, O, H_2O and H_2O_2. Scatter plots of hydroxyl, hydrogen and oxygen resemble each other, related to the chain reaction. The species of HO_2 and H_2O_2 also resemble due to the reactions connecting both the species. The intermediate species are produced strongly under the flame stretch, being attributable to the increase in the coexistence of oxygen and hydrogen.

Conclusions

In order to evaluate the prediction performance of the probability density function method considering a finite chemical reaction rate (F-PDF), a turbulent jet nonpremixed flame of hydrogen/nitrogen was calculated by the F-PDF, the PDF method considering the infinite chemical reaction rate (I-PDF), and the flamelet model (F.M.) method. The primary results obtained are as follows:

1. The F-PDF method is able to predict the quenching based on the flame stretch and the re-ignition downstream of the quenching in turbulent jet nonpremixed flames.
2. The F-PDF method is able to predict the change in the flame structure due to the flame stretch.
3. The F-PDF method predicts the closer maximum temperature to experimental results due to the finite chemical reaction rate.
4. The scalar PDF method underestimates the mixing and leads to higher temperature in the downstream of turbulent jet nonpremixed flames. This deficiency is caused by the present Monte Carlo method.

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